

# **THEORY FACE-OFF**

# ***MOTIVATION AND GROUND RULES***

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- Details of subband energy alignments are expected to be critical factors in device performance for type-II antimonide laser/detector structures
- However, even such fundamental quantity as energy gap tends to vary widely for same structures grown by different growers and under different growth conditions
- Band Structure Face-Off intended to be critical comparison of various theoretical approaches applied to exactly the same three type-II structures: (1) W laser, (2) InAs/GaInSb superlattice detector, (3) InAs/GaSb all-binary detector
- 11 calculations of conduction & valence subband energy levels submitted, based on 3 general approaches: Envelope-function  $k \cdot p$ , Pseudopotential, Tight-binding
- Most calculations employed suggested standard parameter sets for energy gap, effective masses, band offsets, *etc.*, although some participants used their own preferred values

## ***TWO PRIMARY ISSUES***

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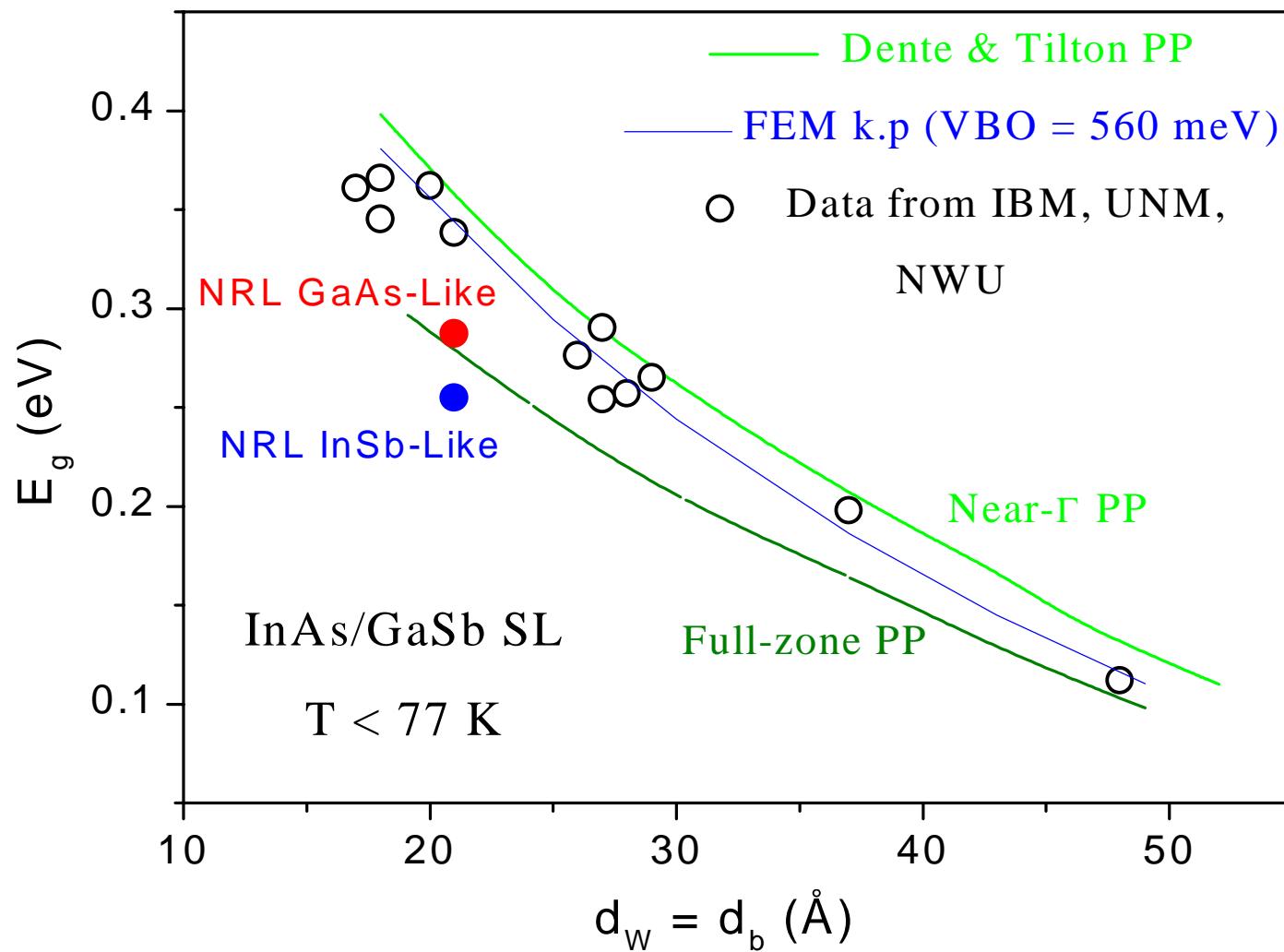
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- Disagreement between experimental and theoretical energy gaps
- Accurate prediction of intervalence energy splittings, to minimize Auger recombination and absorption losses in type-II IR laser and detector designs
  - Almost no directly relevant subband energy data available for guidance

# *COMPARISON OF PL DATA WITH THEORY*

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# **GROWER-DEPENDENT BAND OFFSETS**

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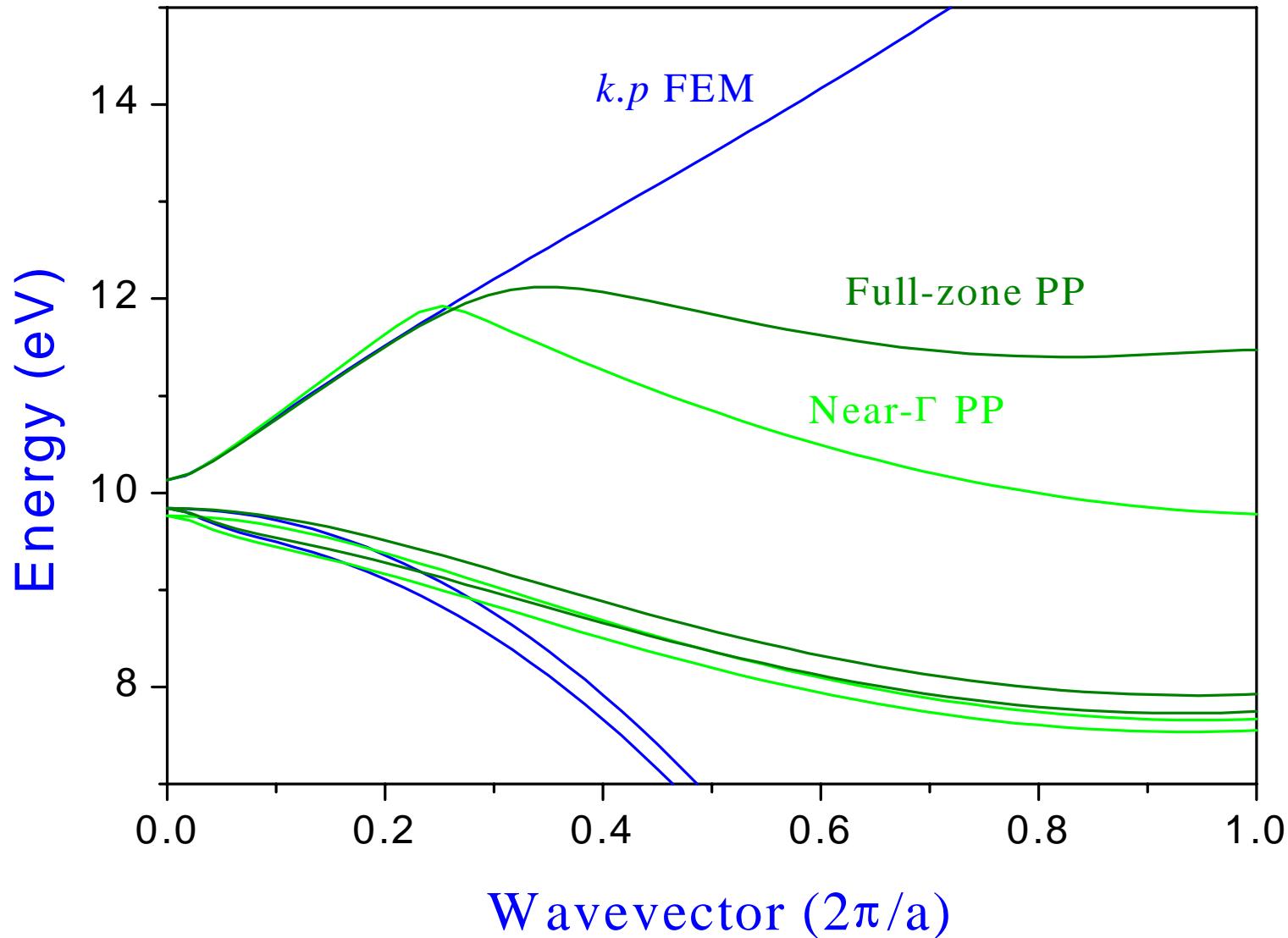


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Grower	Structure	PL Peak Energy (300 K)	Best offset (FEM <i>k.p</i> )
NRL	As/GaInSb/InAs/AlSb W ( $T_s = 400$ °C) 5.5ML/10ML/5.5ML/14ML	280 meV	680 meV
	6/10/6/14	243	700
	7/10/7/14	214	670
	8/10/8/14	183	660
	8/10/8/14 ( $T_s = 450$ °C)	253	610
HRL	InAs/GaSb/InAs/AlSb W	353	650
	InAs/GaSb/InAs/AlSb W	383	650
Sarnoff	W with AlAsSb barrier	354	660
	W with AlSb barrier	413	620
U. Iowa	W with quaternary barrier	310	590
U. Houston	W Laser	282	530
Various NRL	InAs/GaSb SL	100-370	560
	InAs/GaSb SL (InSb-Like)	255	670
	InAs/GaSb SL (InSb-Like)	285	640

# *PSEUDOPOTENTIAL vs $k \cdot p$ FOR **BULK** InAs*

Pseudopotential dispersions from Dente and Tilton (Preliminary)



# *LIST OF PARTICIPANTS*

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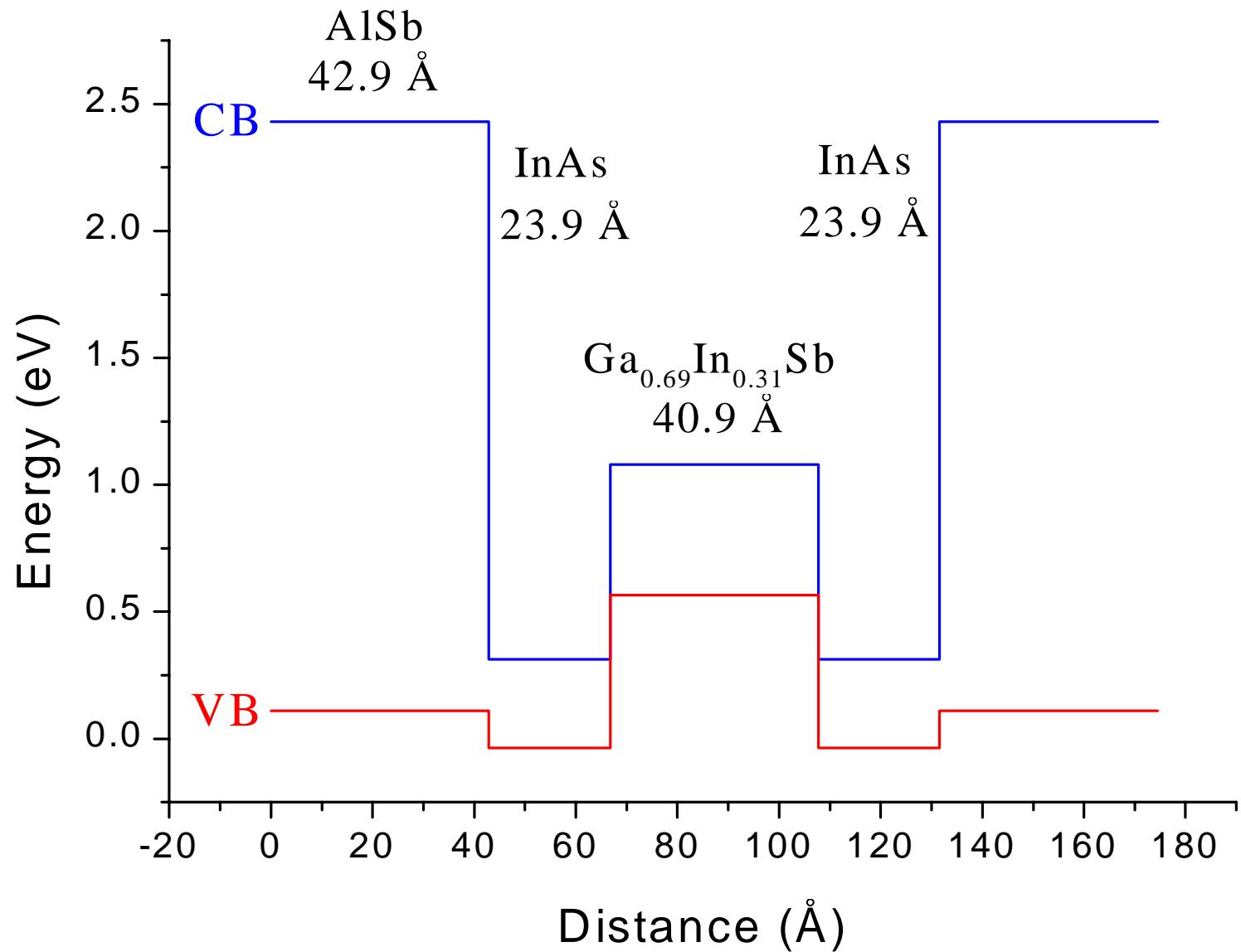
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- I. Vurgaftman, J. R. Meyer (NRL), and L. R. Ram-Mohan (WPI & Quantum Semiconductor Algorithms): 8-band finite-element  $k\bullet p$
- R. Q. Yang and Y.-M. Mu (U. Houston): 8-band finite-element  $k\bullet p$
- J. Zhang and C. H. Lin (U. Houston): 8-band finite-element  $k\bullet p$
- L. T. Heen (NTNU, Norway) and H. P. Hjalmarson (Sandia): 8-band  $k\bullet p$
- F. Szmulowicz (AFRL, Wright-Patterson): 8-band  $k\bullet p$
- M. E. Flatté (U. Iowa): 8-band and 14-band  $k\bullet p$
- G. C. Dente and M. L. Tilton (AFRL, Phillips): Empirical Pseudopotential
- M. J. Shaw and M. Jaros (U. Newcastle): Empirical Pseudopotential
- J. Schulman (HRL): 2-band Tight-Binding
- G. Klimeck (JPL) and T. Boykin (U. Alabama): Tight-Binding
- J. P. Loehr (AFRL, Wright-Patterson): Effective Bond-Orbital (Tight-Binding)

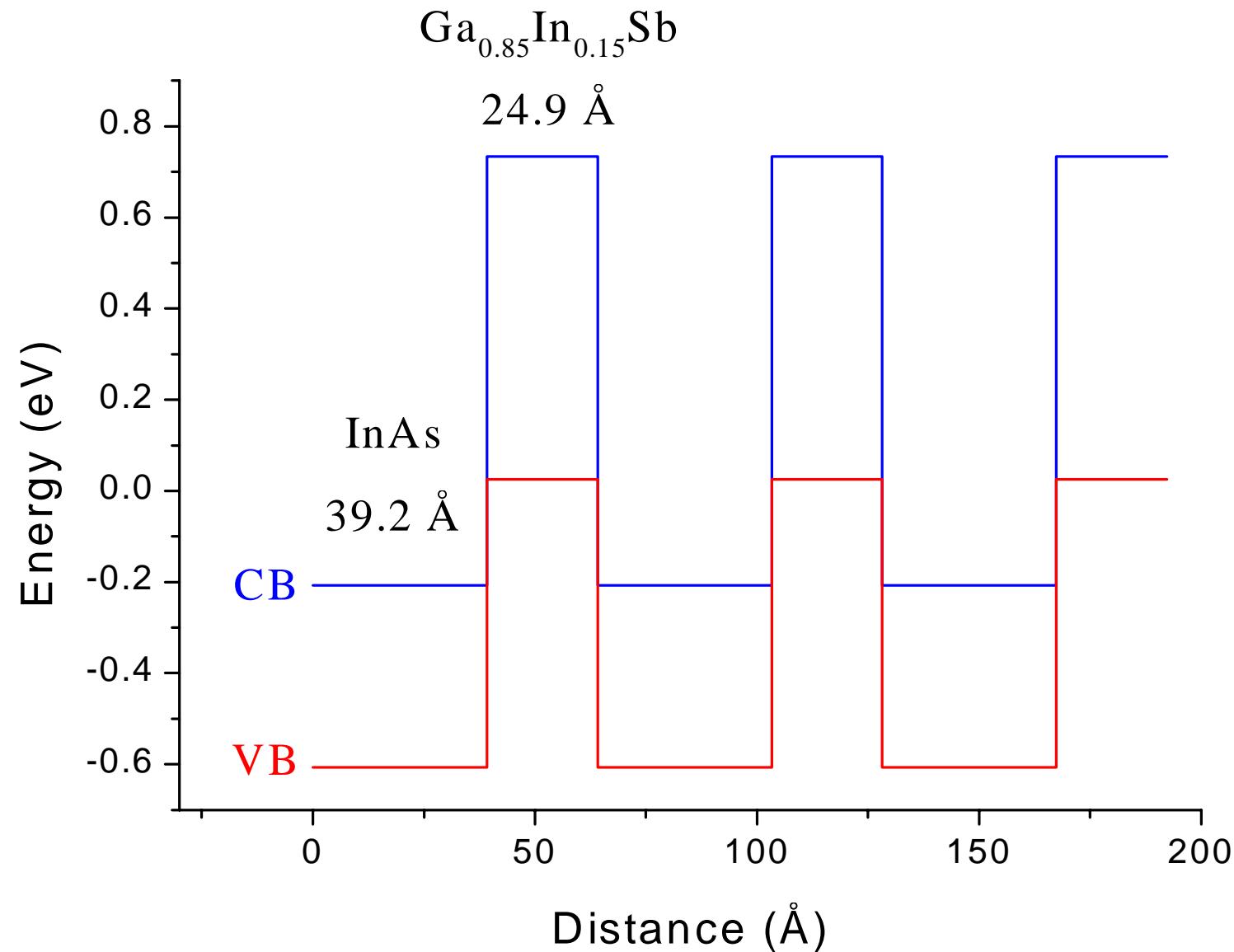
# ***STRUCTURE 1 – W LASER***

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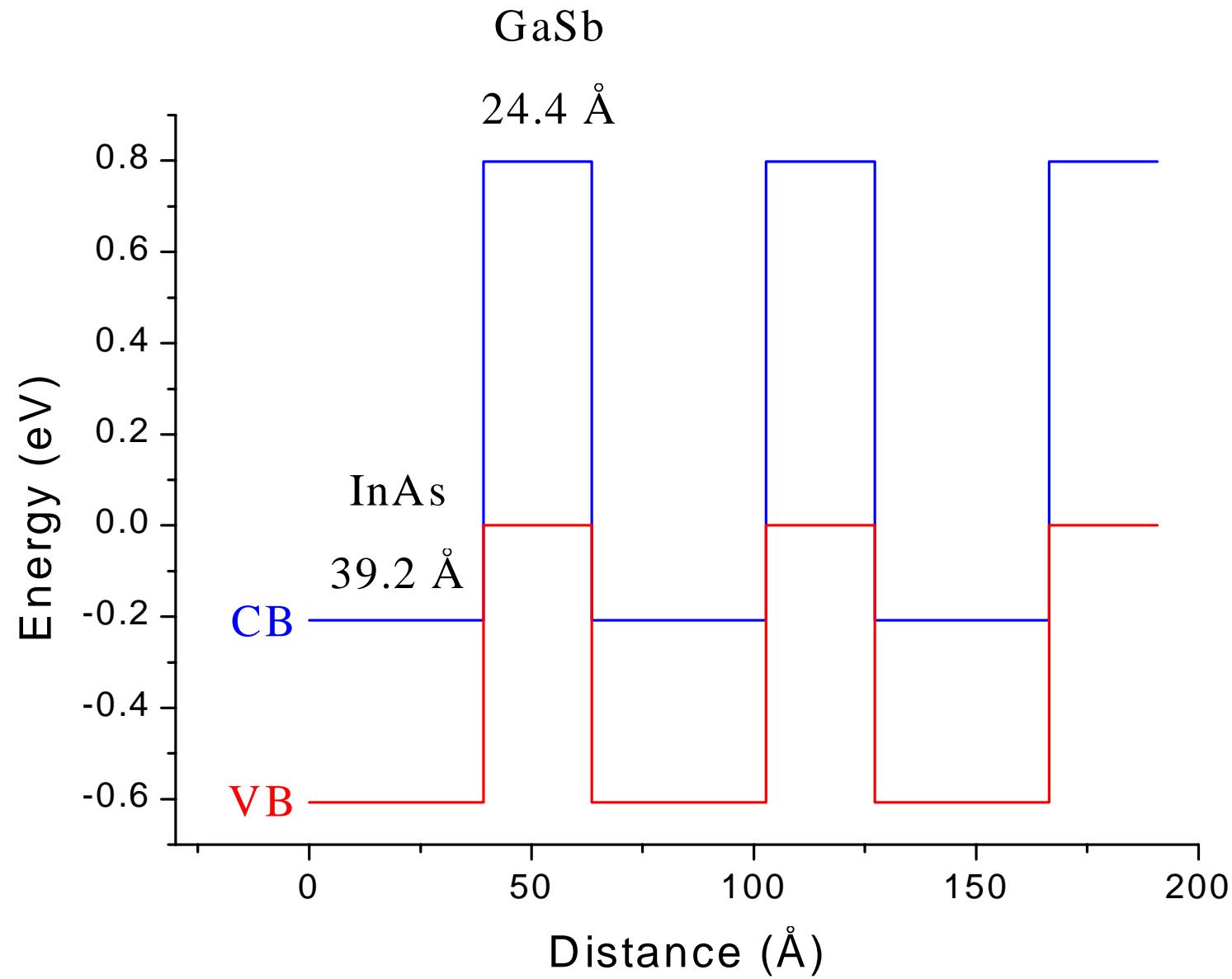
## *STRUCTURE 2 – IR DETECTOR*



# *STRUCTURE 3 – ALL-BINARY DETECTOR*

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# STRUCTURE 2

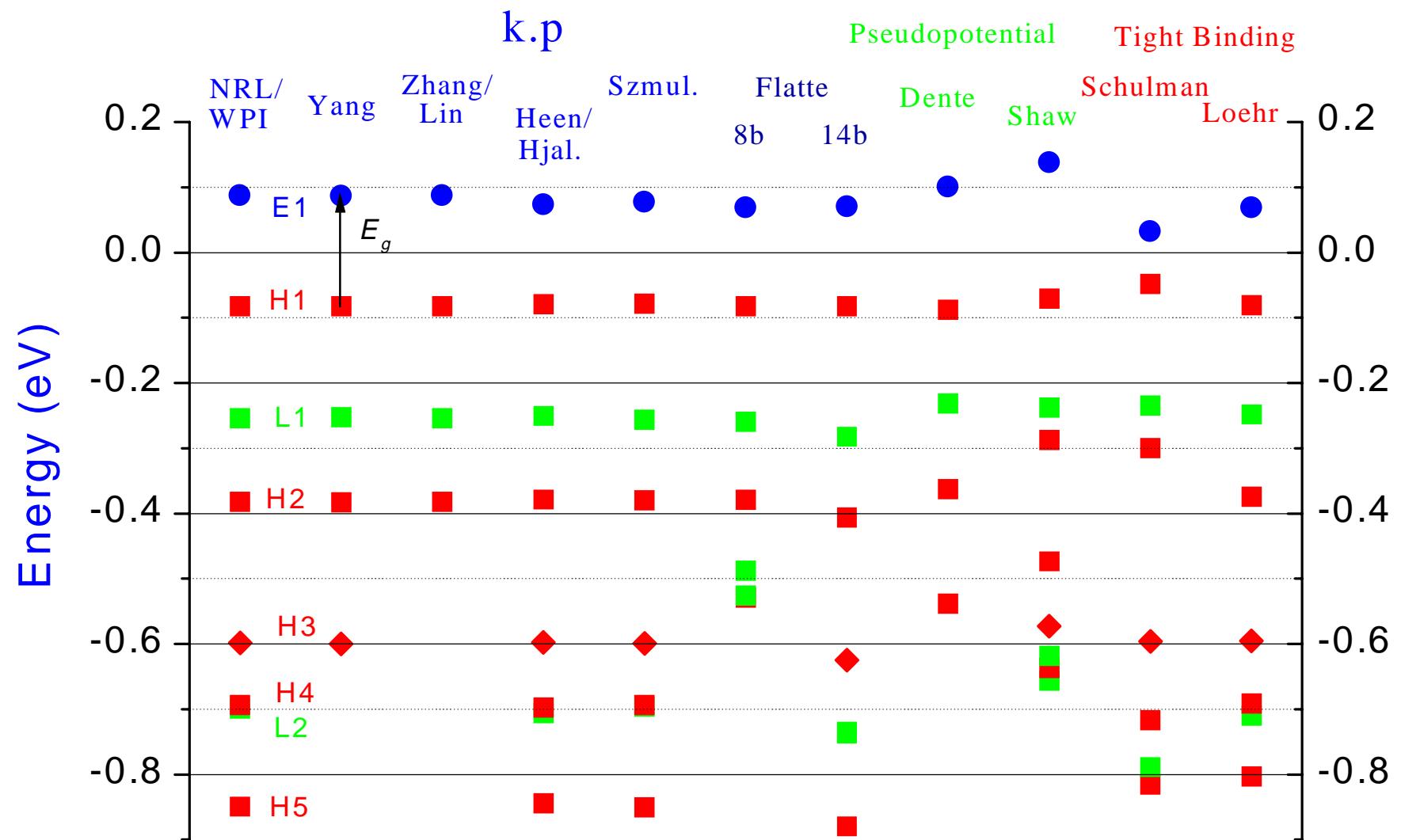
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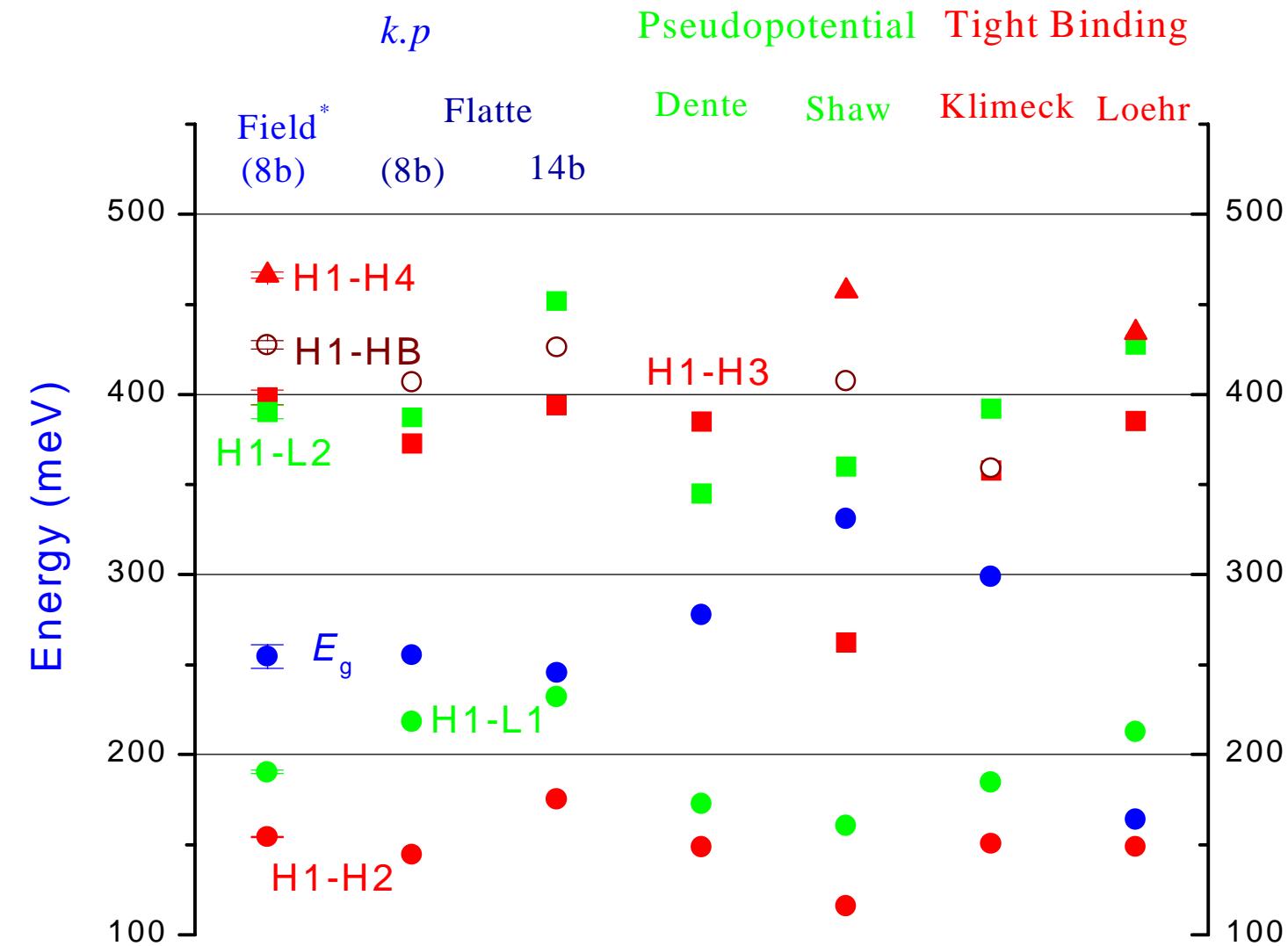
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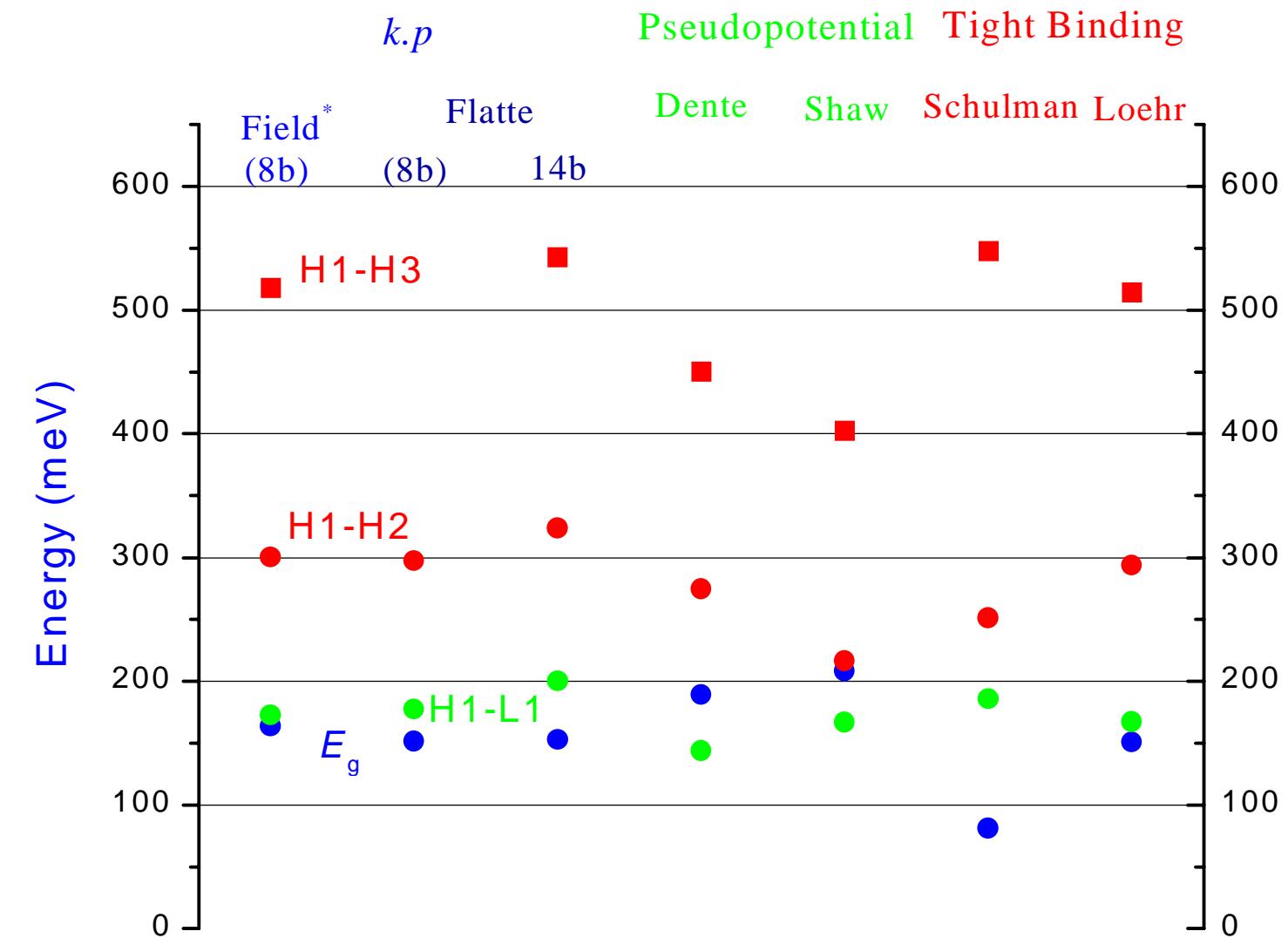


# *STRUCTURE 1*



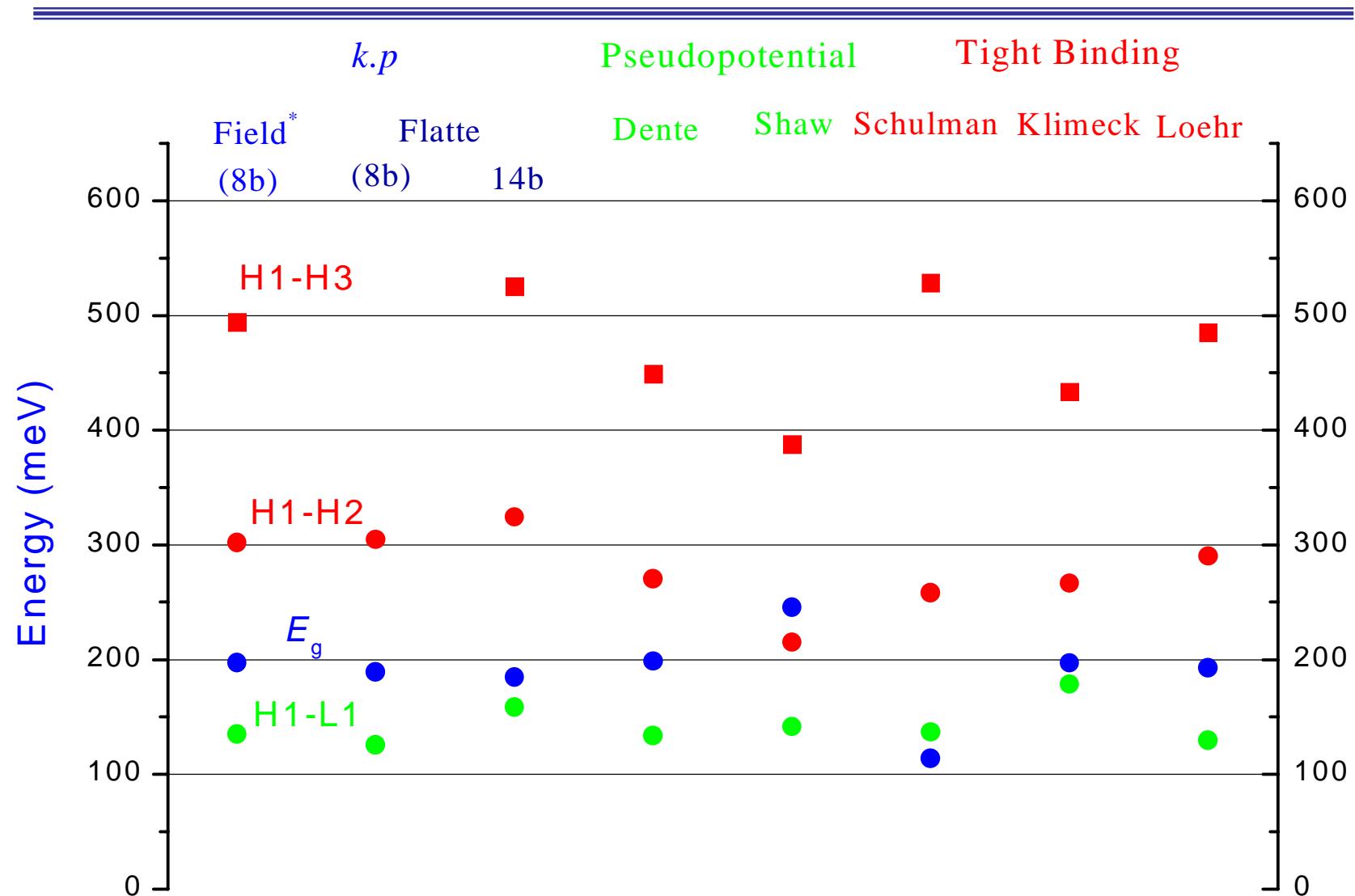
\*NRL/WPI, Yang, Zhang/Lin, Heen/Hjalmarson

# *STRUCTURE 2*



\*NRL/WPI, Yang, Zhang/Lin, Heen/Hjalmarson, Szmulowicz

# ***STRUCTURE 3***



\*NRL/WPI, Yang, Zhang/Lin, Heen/Hjalmarson, Szmulowicz

## ***EFFECT OF INTERFACE BOND TYPE***

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	$E_g$ (InSb) (meV)	$E_g$ (GaAs) (meV)	$E_g$ (1:1) (meV)	$dE_g$ (meV)
Structure 1				
Loehr	140	144.1		4.1
Structure 2				
Loehr	123.4	163.8		40.4
Schulman	89.9	88.2		-1.7
Structure 3				
Loehr	158.6	204.3		40.4
Schulman	121.9	124.1		-2.2
Shaw	218.8		245.4	26.6

# *OBSERVATIONS*

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\*Caveat: Some observations may be anecdotal, due to different parameter sets, other factors

- $k \bullet p$ : Given the same input parameters, calculations gave nearly the same energy gaps and intervalence subband splittings (not surprising, but reassuring)
- Pseudopotential: Larger energy gaps and smaller intervalence splittings than  $k \bullet p$  - Trends similar from two calculations
- Tight-binding: Energy gaps especially variable (both larger and smaller than  $k \bullet p$ ), intervalence splitting comparable to  $k \bullet p$  -- Three calculations sometimes differed widely
- Interface bond type: Pseudopotential and tight-binding calculations imply -2 to 45 meV difference in  $E_g$  for GaAs-like vs InSb-like (Experiments have implied 15-40 meV difference)
- Energy gaps: No single set of parameters accounts for structures from different growers and different growth conditions – Effects of interdiffusion, interface roughness, interface bond type, *etc.*, do not appear large enough to explain
- Intervalence splittings: Systematic difference between different approaches (especially  $k \bullet p$  and pseudopotential) -- Presently no data to determine who is right